PROCESSING OF THE DATA OBTAINED FROM THE POLAROGRAPHIC ANALYZER PRINCETON APPLIED RESEARCH MODEL 384B BY THE PROGRAMMING PACKAGE QPRO

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Voltammetric data obtained from the Polarographic Analyzer Princeton Applied Research Model 384B can be successfully processed by the programming package QPRO. This program enables a numbered graphical presentation of the voltammetric curves and many mathematical and statistical calculations over the tabulated data. Additional processing of the data allows using the analyzer not only for analytical purposes, but also in theoretical investigations and calculation of important kinetic parameters.

Key words: voltammetric data; processing; programming package; QPRO

INTRODUCTION

The polarographic analyzer PRINCETON AP-PLIED RESEARCH MODEL 384B represents a new generation of microprocessor based instruments. It is supplied with RS232 interface for connection with computer and for additional processing of data. The manufacturer offers specialized programming packages only for graphical presentation of the data. The price of these packages is not included in the price of the instrument. A possible way for data processing is the use of the well-known spread-sheet programming package QPRO[1]. This program is one of the best programs in its class and widely used in many fields [1, 2]. These features make it easily accessible and well supported with literature. All these facts support the choice of this program for processing the data from the polarographic analyzer. In this paper, some simple examples for graphical presentation of the voltammetric curves and some mathematical calculations over the voltammetry data are presented.

DISCUSSION

The rear-panel RS232 of the polarographic analyzer is designed to provided for maximum flexibility and utility. This interface is used to drive the plotter or an RS232 compatible device such as printer or computer. The interface RS232 is provided for two-way communication, that is, RS232 used both to send and receive information over a single cable. The RS232 additionally allowed the Model 384B to be controlled from an external device. It may, for example, be routed to a Plotter for obtaining the data in graphic form, or may be routed to a printer for obtain the data in the tabular form. If the communication is achieved with the computer, the data can be presented in the two forms (tabular and graphic presentation) at the same time.

The first step of the communication process is receiving the information from the polarographic analyzer. It can be performed either by a standard MS DOS procedure or by some of the specialized communication packages. This operation can be conveniently done by communication program MODEM that operates under MS-WINDOWS. It has to be taken into consideration that the Model 384B both transmits and receives 8-bites codes. The most significant bit is always "0". The other seven bits are as defined in the ASCII standard. No parity is transmitted. The rate at which the RS232 interface receives data is 2400 baud.

The received data in the text format file has to be converted in the QPRO format file. The conversion of the file can be performed by "Tools" and "Import"

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[1] LONDON BOROUGH OF LAMBETH version 3.00

options. Such a converted file contains a table in which the values of the applied potentials on the working electrode are placed as a first column, and the corresponding currents' data as a second one. Also, the file contains information about the starting and final potentials, the number of the sample and the data about the founded peaks.

The "Graphic" option enables numerous ways of graphical presentation of the *E-i* curves. The most usual manner is plotting of the potentials data against the current values. The various voltammetric curves of 6-propyl-2-thiouracil recorded in Britton-Robinson buffer at pH=3 are shown in the Fig. 1. It can be seen that there is a primary and a secondary Y-axis. This capability provides for presentation of a various type of voltammetric curves, which are quite different in their currents' values (for example: the low sensitive dc polarography and the very high sensitive square-wave voltammetry) on the same graphic. The final arranging of the graphic (writing of the text in the graphic area, drawing the various tapes of marks for emphasizing of the important part of the graphic, etc.) can be performed by "Graphic" and "Annotated" options. In Fig. 2 the six SW-voltammetric curves are presented on the same graph. With this type of graphical presentation, the effect of some experimental condition (for example the effect of the various accumulation times, temperature, concentration, etc.) on the voltammetric curves, can be emhasized.

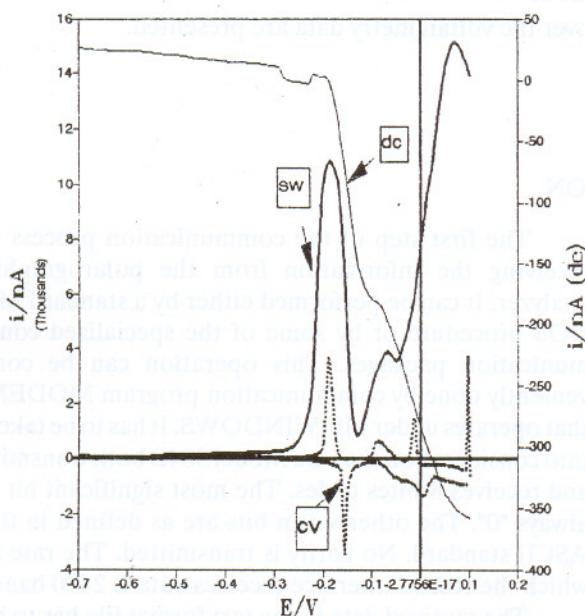The powerful graphical presentation of the data is only a part of the capability of the QPRO. The
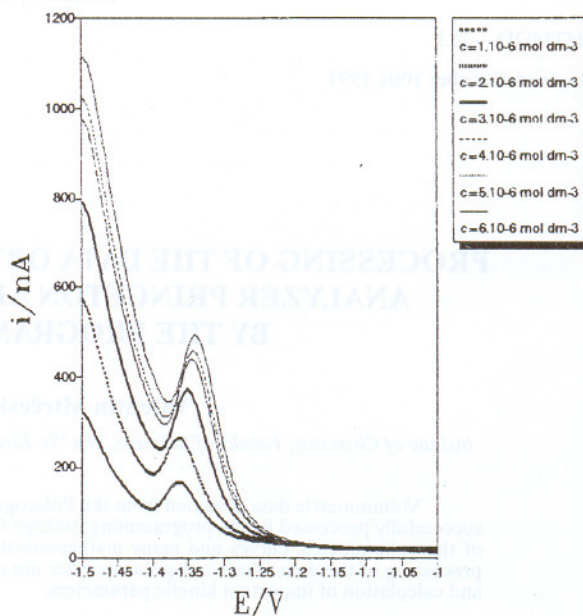

Fig. 2. Graphic presentation of the six same-tape of voltammetry curves recorded during the variation of one experimental parameter (in the concrete case, the increasing of the concentration of analyte). From such graphic it is obvious how the voltammetry curves depend on the investigated experimental parameter.

program offers a various mathematical manipulation under tabulated data. In Fig. 3 the subtraction process of one curve from another is presented. Such an operation can be usefully exploited for presentation the difference between the "sample" and the "blank" curve, or for a precise quantitative measurements.

The option "Tools" and "Advanced Math." offers some standard mathematical operations. Some of them are the regression analysis and solving of the equations. Also, there is a possibility to examine the result of some equation under variation of its two variables (some kind of a fitting process). For example, the regression analysis performed under logarithmic trasformed values of the rising portion of the dc polarographic wave (Fig. 4), results in a straight line. The slope of this line is determined by the reversibility of the electrode process. In some cases, the slope of the regression analysis curve reveals the number of the electrons that are included in the electrode reaction.

The calculation of the important kinetic parameter α can be performed in various ways. According to the theory for dc polarography [3, 4], the kinetic parameter α is defined by the equation

$$\alpha = RT/n\Delta E \cdot \log[\,(i_d - i)/i\,]$$

The inputing data from the rising portion of the dc polarogram in the above equation, yields with a series of values for α. The value for the average transition coefficient α, can be easily calculated by

Fig. 1. Graphic presentation of the tree tape voltammetric curves. This tape of graphics reveals much more information about the electrode process. The secondary Y-axis is related to the low sensitive dc polarography.
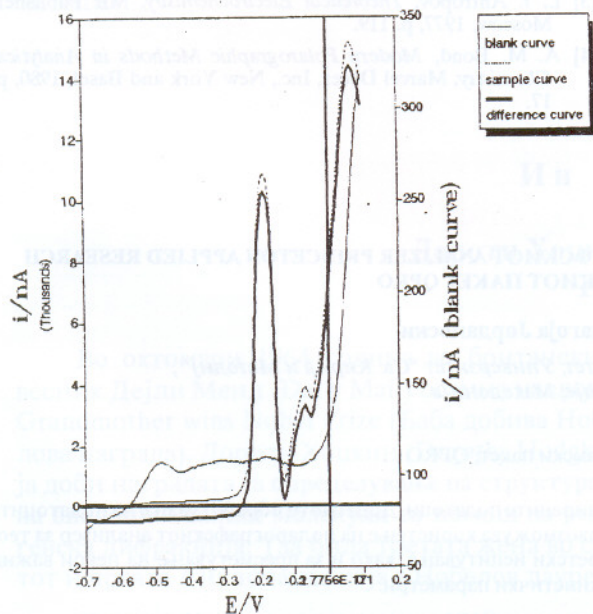
Fig. 3. Graphic presentation of the subtraction process between the "sample" and the "blank" voltammetry curves. The resulting curve avoids the effect of the supporting electrolyte
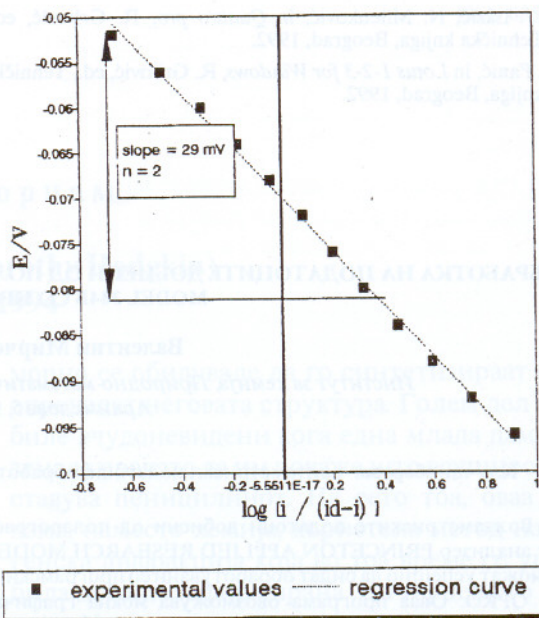

Fig. 4. The regression analysis curve performed on the data from the analysis of the reversibility of the electrode process. The slope of the regression analysis curve is determined by the reversibility of the electrode process and the number of the electrons included in the electrode reaction.

applying the statistical function "AVRG." Also, the calculation of this parameter can be performed starting from the mathematical definition of the dc wave for an irreversible electrode process:

$$E = E_{1/2} + RT/n \, \alpha \, F \cdot \log\left[(i_d - i)/i\right]$$

The options "Tools" and "Solve for" are able to calculate the values of the transition coefficient α. For these purposes, the values of the potentials from the rising portion of the dc wave have to be inputed on the left-hand side of the above equation. The solving of this series of equations for the unknown variable α by the option "Solve for" yields the numerical values of the transition coefficient α.

The effect of the various values of the coefficient α on the dc waves is presented in Fig. 4. It is obvious that in the particular case the best coinciding between the calculated and experimental values exists when the average transition coefficient α is 0.45. Such investigation is performed by solving the equation

$$i = i_d / \left[\exp(\Delta E \, \alpha \, nF)/0.434RT + 1\right]$$

for various values for α. That process can be easily performed by using the "Tools" and "What if" option.

The presented examples show a simple way for calculation of some important kinetic parameters. The above presented results performed by additional processing of the voltammetric data by programming
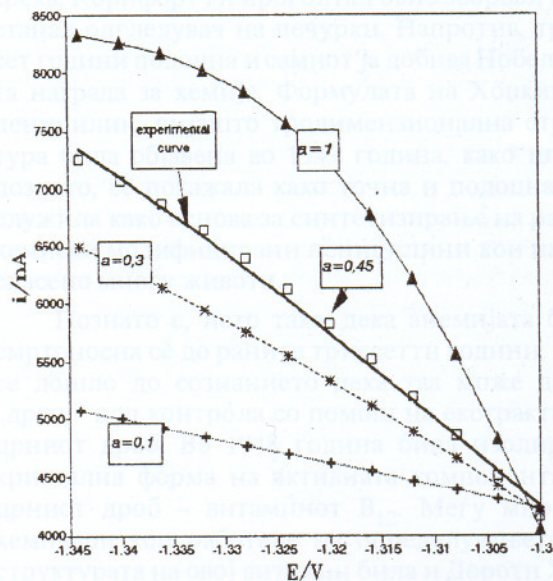

Fig. 5. Correlation between the experimental and calculated dc-currents values. The calculations were performed under various values for the kinetic parameter α. From the graphic, it's obvious that the kinetic parameter α in the concrete case is about 0.45.

package QPRO extents the field of application of the polarographic analyzer to the theoretical investigations.

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Р е з и м е

ОБРАБОТКА НА ПОДАТОЦИТЕ ДОБИЕНИ ОД ПОЛАРОГРАФСКИОТ ANALIZER PRINCETON APPLIED RESEARCH MODEL 384B СО ПРОГРАМСКИОТ ПАКЕТ QPRO

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Клучни зборови: волтаметриски податоци; обработка; програмски пакет; QPRO

Волтаметриските податоци добиени од поларографскиот анализер PRINCETON APPLIED RESEARCH MODEL 384B можат успешно да бидат обработувани со програмскиот пакет QPRO. Оваа програма овозможува моќна графичка презентација на волтаметриските криви, како и извршување на различни математички и статистички пресметки на табелираните податоци. Додатното обработување на податоците овозможува користење на поларографскиот анализер за теоретски испитувања, како и за пресметување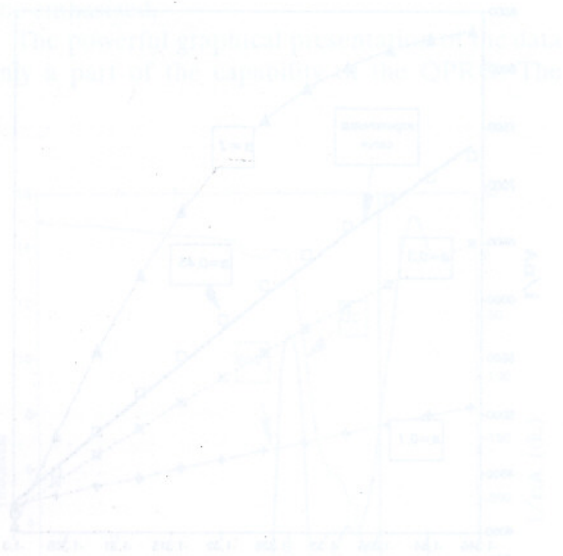 на некои важни кинетички параметри.